

# The 1D $t$ - $J$ model with next-nearest neighbor hopping - breakdown of the Luttinger liquid?

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We investigate the effect of a next-nearest neighbor hopping integral  $t'$  in the 1D  $t$ - $J$  model, using Lanczos diagonalization of finite chains. Even moderate values of  $t'$  have a dramatic effect on the dynamical correlation functions and Fermi surface topology. The high-energy holon bands become diffuse and overdamped, the band structure near the Fermi energy is dominated by  $t'$ . With increasing hole concentration the system undergoes a phase transition which changes the volume of the Fermi surface, but neither phase has a  $k_F$  compatible with a Luttinger liquid.

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One dimensional (1D) systems of interacting Fermions have been the subject of much interest over many years. Based on the results of exact solutions for some models [1,2] and approximate techniques, such as Bosonization [3] or the renormalization group [4], the belief has formed that the universal fixed point model for systems with a repulsive interaction between the Fermions is the Luttinger liquid. Key features of this exotic quantum liquid are the existence of ‘noninteracting’ collective spin and charge like excitations, the so-called spinons and holons, which usually have different velocities, and the two Fermi points which obey the Luttinger sum-rule and govern the low energy physics. In the following, we want to present numerical evidence indicating that a very simple (and actually quite “physical”) model, the 1D  $t$ - $J$  model with next-nearest neighbor hopping, may not fall into the class of the conventional Luttinger liquid. More precisely, the model reads:

$$H = - \sum_{i,\sigma} [ t \hat{c}_{i,\sigma}^\dagger \hat{c}_{i\pm 1,\sigma} + t' \hat{c}_{i,\sigma}^\dagger \hat{c}_{i\pm 2,\sigma} ] + J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}.$$

Here  $\hat{c}_{i,\sigma} = c_{i,\sigma}(1 - n_{i,\bar{\sigma}})$  and  $\vec{S}_i$  denotes the spin operator on site  $i$ . Throughout we keep the values  $t=1$  and  $J=0.2$  (although the results do not depend on this special choice).

In the “ordinary”  $t$ - $J$  model the combination of hard-core constraint and one-dimensionality obviously does not allow the sequence of spins along the chain to be changed by the motion of holes. The factorization of the wave function into a charge and spin part [5] then appears as a quite natural consequence. Introduction of next-nearest neighbor hopping changes this, in that hopping alone now can interchange spins. Obviously, this re-introduces some coupling between spin and charge degrees of freedom, but the question is whether this coupling does not simply “renormalize to zero” in the actual ground state. We tried to address this question by studying various dynamical correlation functions, computed numerically by Lanczos diagonalization of small clusters [6]. It turned out that even for quite moderate values of  $t'$  the cou-

pling of spinon and holon is large and in fact seems to be strong enough to induce a breakdown of the Luttinger Fermi surface.

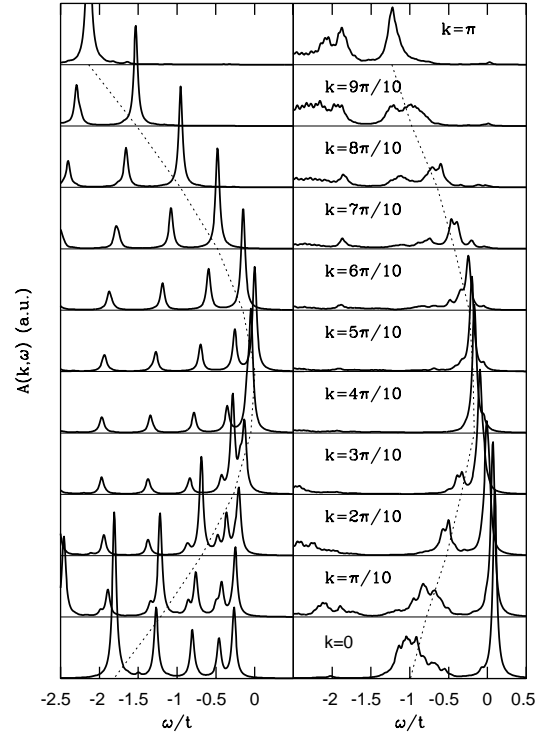


FIG. 1. Electron removal spectrum for a half-filled 20-site ring with  $t' = 0$  (left) and  $t' = -0.4$  (right). The dotted line indicates the “holon band”.

To begin with, we consider the electron removal spectrum at half-filling shown in Figure 1. Introduction of even a rather small  $t'$  has a quite significant effect on the spectrum. For  $t'=0$  the spectrum consists of a sequence of sharp peaks, which actually form a very systematic network of “spinon and holon bands” [7]. The topmost band for  $k \leq \pi/2$  traces out the spinon dispersion, and consequently its bandwidth scales strictly with  $J$ , the topmost band for  $k > \pi/2$  follows the holon dispersion [7].

In the spectrum for  $t' \neq 0$  some diffuse remnant of the “holon band” can be identified, but it no longer has the character of a well-defined excitation. The smaller peaks at higher excitation energies, which were sharp and had a well-defined dispersion for  $t'=0$ , disappear completely. Obviously the coupling of spin and charge degrees of freedom due to  $t'$  induces a strong damping of the holon. Next, the uppermost band between  $k=0$  and  $k=\pi/2$  has inverted dispersion, so that its top now is at  $k=0$ . A more detailed study of this “quasiparticle band” for different  $t'$  (see Figure 2) shows that its dispersion is determined by  $t'$ . The width of this band, defined as  $W = \epsilon(0) - \epsilon(\pi/2)$  can be fitted well by the expression  $W(t') = 1.2 \cdot (J + t')$ . Its dispersion on the other hand seems to change from nearest neighbor hopping,  $\epsilon(k) \propto \cos(k)$  to next-nearest neighbor hopping,  $\epsilon(k) \propto \cos^2(k)$  for larger  $t'$ . This shows that the character of this band must be very different now in that its

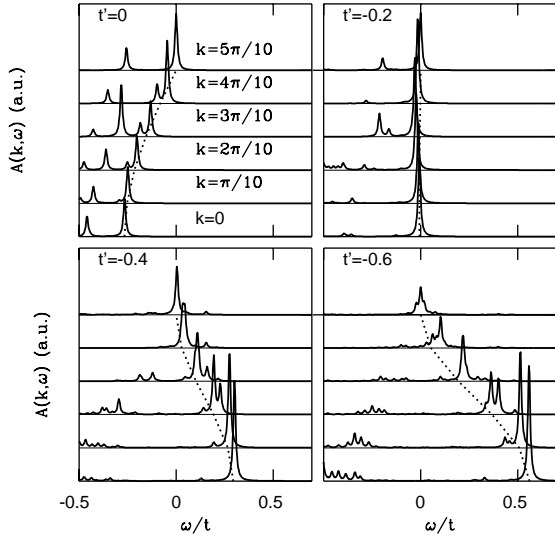


FIG. 2. “Quasiparticle band” in the electron removal spectrum of a half-filled 20-site ring with different values of  $t'$ . The dotted line gives the curves  $\epsilon(k) = W(t') \cos(k)$  for  $t' = 0, 0.2$ , and  $\epsilon(k) = W(t') \cos^2(k)$  for  $t' = 0.4, 0.6$

dispersion is determined by a combination of the exchange constant (which acts only on the spin degrees of freedom) and the next-nearest neighbor hopping integral (which acts on the charge degrees of freedom). Already this simple comparison thus demonstrates that the  $t'$ -term has a surprisingly strong effect.

We proceed to the doped case and study the spin and charge-density correlation function, shown in Figure 3. The density correlation function (DCF) shows a striking difference between the case  $t'=0$ , where it consists of a series of sharp dispersive peaks, and the case  $t'=-0.4$  where the peaks are replaced by structureless continua. It is only at very low excitation energies that there are sharp peaks also for nonvanishing  $t'$ , the lowest of them appearing at  $k_{0,c}=2\pi/8$ . Again, we see the strong damping of the holon introduced by  $t'$ . On the other hand,

the spin correlation function (SCF) does show some well defined peaks. A major difference is the very small energy scale of the SCF for  $t'=-0.4$ . After rescaling excitation energies, however, there is a certain similarity with the SCF for  $t'=0$ . One can still recognize a series of faint peaks which trace out the “spinon arc” [2] and take their minimal excitation energy at  $2k_F=7\pi/8$ . These peaks, however, correspond in fact to relatively high excited states, and the lowest peak, which also has a much higher intensity, now occurs at  $k_{0,s}=\pi/8$ . As would be the case in a conventional Luttinger liquid [2] we thus have  $k_{0,s}=k_{0,c}/2$ , which interpretation however would force us to choose  $2k_F=\pi/8$ , corresponding to a Fermion density of  $1/8$ , i.e. the density of holes in the

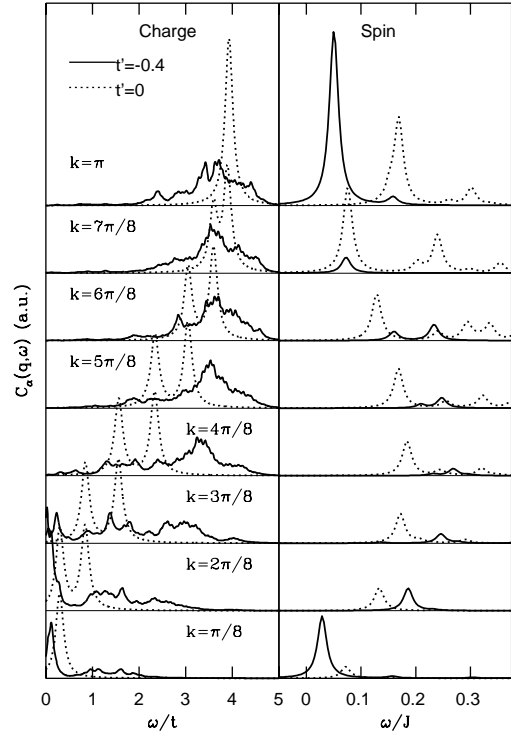


FIG. 3. Dynamical spin and charge correlation function for a 16-site ring with two holes with  $t'=0$  (dotted line) and  $t'=-0.4$  (full line). Excitation energies for the SCF at  $t'=0$  are multiplied by 0.12.

half-filled band. To further address this surprising result, we proceed to the complete single-particle spectral function, shown in Figure 4 for different hole number. We begin with the case of two holes (left hand panel) and focus on energies around  $E_F$ . There, the “quasiparticle band” persists with nearly unchanged spectral weight and dispersion, and the chemical potential essentially cuts into this band to form a hole pocket at  $k=0$ . While the qp-peak at  $k=0$  crosses completely to the inverse photoemission side, there is also some low intensity IPES weight at  $k=\pi/8$ , which probably corresponds to the standard “smearing” of the Fermi surface due to interactions. Doping two holes into the system shifts one

$k$ -point (namely  $k=0$ ) through the chemical potential; this implies that the doped holes act as spin-1/2 particles, leading to the “effective” Fermion density 1/8,

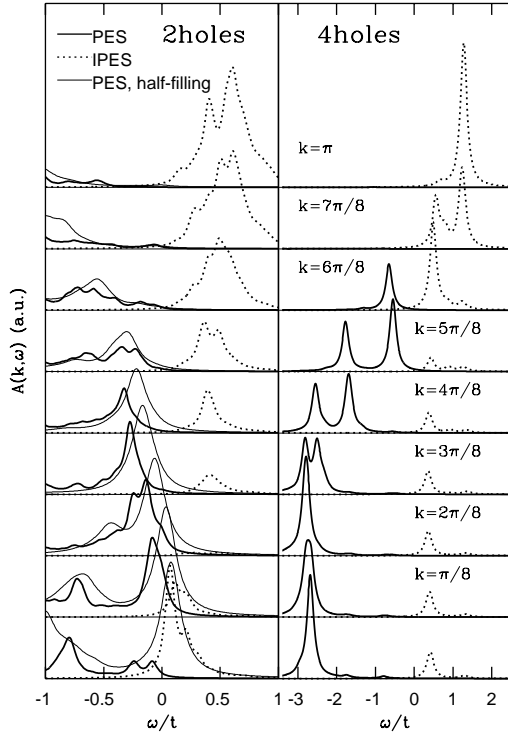


FIG. 4. Full single particle spectral function for a 16-site ring. The chemical potential, defined as being halfway between the excitation energies of first ionization and first affinity state, is the zero of energy,  $t' = -0.4$ .

in complete agreement with the  $k_F$  inferred from the correlation functions. On the other hand, there are also deviations from pure rigid-band behaviour: starting at approximately  $3\pi/8$  there appears a broad high-energy band at an excitation energy of approximately  $0.5t$  in the inverse photoemission spectrum. This “band” has virtually no dispersion, but is spectral weight increases continuously with  $k$ . It never even approaches the Fermi energy and thus is obviously unrelated to any “Fermi surface physics” (this is also confirmed by the ground state momentum distribution, which decreases slowly and completely continuously for  $k > 2\pi/8$ ). It should be noted that the appearance of considerable electron addition weight in the outer part of the Brillouin zone is an essentially trivial property of any Hamiltonian with a dominant nearest-neighbor hopping term: it is simply a necessary condition for having negative kinetic energy [8]. In the 2D model this high energy inverse photoemission weight in the outer half of the Brillouin zone can be explained by “charged magnons”, i.e. spin excitations which previously formed the dressing cloud of the annihilated hole [9]. It is quite plausible that the diffuse high energy band in the present case is of a similar origin. While the spectral function for two holes thus shows

rather clear rigid-band behaviour (at energies close to  $E_F$ ) the situation changes completely for 4 holes (see the right panel of Figure 4). To begin with, unlike the two-hole case where  $A(\vec{k}, \omega)$  had extended incoherent continua, the spectral weight is now concentrated in very few sharp peaks (for graphical reasons we have used different Lorentzian broadenings and  $y$ -axis scales in the two panels of Figure 4; in reality, the weight of the peaks in the right hand panel is about 5 times higher than those in the left-hand panel). These peaks form an almost dispersionless band near  $k=0$ , which then splits into two bands. These cross the Fermi energy separately and “recombine” at  $k=\pi$ . The picture is somewhat unclear in that there is also a dispersionless “band” of low intensity peaks in the electron addition spectrum, which skims just above the chemical potential. We have scanned a variety of hole numbers  $N_h$  and chain lengths  $N$  and always found either one of the two types of spectra in Figure 4; more precisely, for  $N_h/N=2/14$ ,  $2/16$ , and  $2/18$  we found a spectral function as in the left panel of Figure 4, whereas for  $N_h/N=2/12$ ,  $4/14$ ,  $4/16$  and  $6/16$  we found that the spectral function looks like the right hand panel of Figure 4. This indicates that the very different shape of the two spectra does not originate from some spurious commensurate ordering, which would occur only for one special value of  $N_h/N$ ; neither can it be due to a low spin-high spin transition, because all ground states under consideration are spin singlets. Rather, the only relevant quantity determining which spectrum is observed is the hole density, with the critical density  $\delta_c$  for the crossover being  $1/7 < \delta_c < 1/6$ . We thus have a concentration dependent phase transition between two ground states of very different nature. While details of the phase diagram will be reported elsewhere, we also note that for both high and low doping region the phase transition to the ‘anomalous’ phases occurs for  $|t'| \approx J$  (the precise value depends somewhat on  $J$ , being smaller for large  $J$ ; both transitions can be clearly identified by a pronounced change of the electron momentum distribution). The close relationship of the ‘critical’  $t'$  with  $J$  also shows that the transitions are *not* driven by a deformation of the noninteracting band structure. We have observed the transition to the ‘hole pocket’ phase also in the Hubbard model with next-nearest neighbor hopping as  $U$  increases; this also will be reported elsewhere. We still investigate in more detail the properties of the high doping phase. Figure 5 shows the development of the spectral function for increasing hole concentration.  $A(\vec{k}, \omega)$  behaves very similar to that of noninteracting electrons, with the chemical potential progressively cutting more and more into an almost rigid “band”. The only exception is the dispersionless low intensity peaks in the addition spectrum, which seems “pinned” to the chemical potential. However, there is a very significant difference as compared to ordinary electrons. Inspection

of the sequence  $N_h=4, 6, 8$  shows that removing two electrons from the system shifts the Fermi momentum by  $\pi/8$ . On the other hand, to shift  $k_F$  by this amount for spin-1/2 particles would require to remove 4 electrons (namely one electron/spin direction at  $\pm k_F$ ). In fact, counting those momenta where PES and IPES spectrum have a strong low energy peak (such as  $6\pi/8$  in the 4 hole case) as “half-occupied”, the number of momenta in the unoccupied part of the band equals  $N_h$  for  $N_h \geq 4$ . We thus arrive at the conclusion that the doping dependence of the spectral function in the high doping phase is consistent with holes behaving as spinless Fermions.

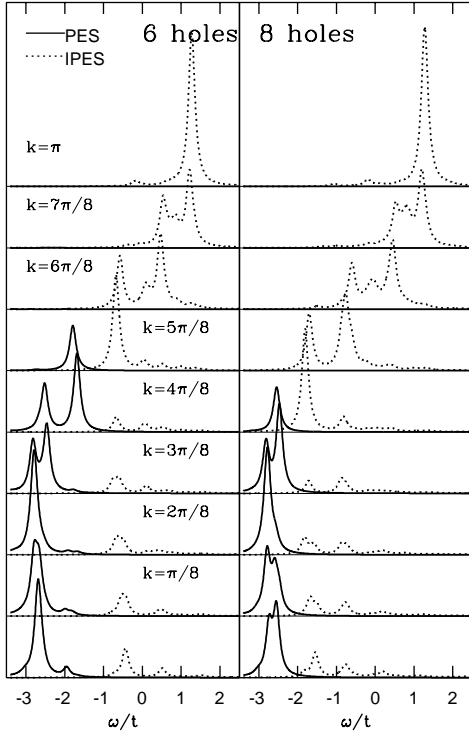


FIG. 5. Full single particle spectral function for a 16-site ring. Parameter values as in Figure 4.

In summary, we have studied the 1D  $t$ - $J$  model with an additional next nearest neighbor hopping integral  $t'$ . As a surprising result, the physics of the model seems to change completely already for moderate values of  $t'$ . In particular the data suggest a phase transition between phases of different Fermi surface volume. Thereby the low doping phase shows quite some similarity with the case of 2D, but also with doped  $t$ - $J$  ladders: the “holon” excitation is overdamped, the single particle spectral function [7] and the density correlation function [10,11] consist of sharp low energy peaks and structureless continua at high energies. Upon doping the spectral function shows rigid-band behaviour [12], with the chemical potential cutting into the quasiparticle band seen at half-filling. The Fermi surface takes the form of a hole-pocket [13,14]. The location of the pockets is shifted to

$k=0$ . As the density of holes exceeds a critical value  $\delta_c \approx 0.15$ , there occurs a phase transition to a different ground state. The spectral function now shows a well defined band of sharp dispersive peaks, the doping dependence is consistent with the doped holes being spinless Fermions which gradually occupy this band. The relation between electron density  $\rho_e$  and Fermi momentum  $k_F$ , being  $k_F = \frac{\pi}{2}(1 - \rho_e)$  in the low doping phase and  $k_F = \pi(1 - \rho_e)$  for high doping, is therefore never consistent with the value for the Luttinger liquid, where it is  $k_F^0 = \frac{\pi}{2}\rho_e$  (it has to be kept in mind that the exact-diagonalization technique is hampered by the coarseness of the available momentum and energy resolution; however, the Fermi momenta are quite unambiguously distinguishable in the data and such *qualitative* results are not likely to be prone to finite-size effects). This result indicates a very profound reconstruction of the electronic structure as compared to the conventional Luttinger liquid. It also implies that these phases are not accessible (and hence have not been found previously) by standard methods for discussing 1D systems, such as Bosonization [3] or renormalization group calculations [4]. Both methods start out from the noninteracting Fermi points at  $\pm \frac{\pi}{2}\rho_e$  and attempt to construct effective Hamiltonians for the low energy excitations around these. While the resulting ground state is qualitatively quite different from the noninteracting Fermi sea, it still “inherits” the period of its long range phase coherence, i.e. the correlation function  $\langle c_{i,\sigma}^\dagger c_{j,\sigma} \rangle \propto \sin(k_F^0|i - j|)$ . Anticipating that the Fermi momenta of the two phases of the  $t$ - $t'$ - $J$  model are indeed as discussed above, it is then the period of the long range oscillations of this correlation function are different, although the exponents for its decay are probably again consistent with “modified Luttinger liquids”.

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